

A selection principle in deformation quantization

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Deformation quantization produces families of mathematically equivalent quantization procedures from which one must select the physically meaningful ones. As a selection principle we propose that the procedure must allow enough ‘observable’ energy distributions, i.e., ones for which no pure quantum state will appear with negative probability and must further have the property that for these the uncertainty in the probability distribution of the quantum states must not exceed that of the original distribution. For the simple harmonic oscillator we show that this allows only the classic Groenewold-Moyal (skew-symmetric) form.

The idea of negative probabilities is not new, going at least as far back as Wigner and perhaps even into the 19th century. It has been likened popularly to observers on the sidelines of a soccer game seeing (non-negative) probability distributions of the coordinates of the ball, none of which may seem unusual, but from which they deduce that the probability distribution of the ball over the interior of the entire playing field has points where it is negative. Suppose, however, that we have a system for which we know some distribution of energies. Deformation quantization generally produces a family of ‘cohomologically equivalent’ quantizations of the system, each of which together with the energy distribution assigns a probability, possibly negative, to each pure quantum state. An energy distribution will be called *observable* with respect to a given quantization procedure if each of these probabilities is in fact non-negative. We will say that there are *enough* observable distributions if every distribution is in the closure of the linear space spanned by the observable ones.

With any quantization procedure one can associate to the original distribution of energies two measures of uncertainty (=standard deviation), that of the original distribution and that of the distribution of energies it produces in the various pure quantum states. The latter will be called the *quantum uncertainty*; The selection principle proposed here is that amongst cohomologically equivalent quantizations only those are physically meaningful for which there exist

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enough observable distributions, and where for each observable distribution the quantum uncertainty does not exceed that of the original distribution; briefly *quantization must decrease uncertainty*.

In the case of the simple harmonic oscillator, examining the entire family of quantizations possible through deformation yields identities involving Laguerre polynomials which, aside from the present method of derivation, are generally not new. They show, however, that for each of these quantizations there is a natural infinite sequence of ‘basic’ observable distributions from which any pure state can be recovered as a linear combination. In particular there are always enough observable distributions, so for the simple harmonic oscillator this by itself is no restriction on deformation quantization. However, the only quantization that the inequality on uncertainties allows is the Groenewold–Moyal form (although the normal or anti-normal form may be meaningful when quantizing fields). To single out that form in the case of the simple harmonic oscillator it would be sufficient, as will be shown, to require that the quantum uncertainty of an observable energy distribution approach that of the original distribution as the energy tends to infinity; perhaps this alone would be sufficient in general.

1 Some basic algebraic deformation theory

The seminal paper in deformation quantization is that of Bayen, Flato, Frønsdal, Lichnerowicz and Sternheimer [1] 1978, some essential ideas and results of which are simply reproduced here without further attribution. This approach to quantization has been exceedingly fruitful. Some of the subsequent developments are summarized in [2], which is complemented by an extensive bibliography. (A useful recent introduction to the theory is the note of Hirshfeld and Henselder [5].) We begin with a very brief review of algebraic deformation theory, introduced by the author in [3].

Let \mathcal{A} be an algebra which here (and generally in any physical theory) will be assumed to be over the real or complex numbers, e.g., the algebra of functions on a phase space, but in a more general context could be over an arbitrary commutative, unital ring. A *deformation* of \mathcal{A} is a new associative ‘star’ multiplication expressible as a formal power series

$$a * b = ab + \hbar C_1(a, b) + \hbar^2 C_2(a, b) + \dots \quad (1)$$

Here \hbar is for the moment just a formal parameter and the C_i are bilinear maps from $\mathcal{A} \times \mathcal{A}$ to \mathcal{A} . We should like the star product to be defined on the same underlying vector space as \mathcal{A} but the introduction of the formal parameter \hbar generally makes it necessary to extend the coefficients. Frequently the extension is to power series in \hbar and one views the functions C_1, C_2, \dots as having been extended to be bilinear not only over \mathbb{R} or \mathbb{C} but also over these power series. Often one tacitly assumes this done and in favorable cases the series actually converge for sufficiently small values of the variable \hbar . In deformation quantization, however, this extension of coefficients is not appropriate because we are

forced to consider power series in $1/\hbar$. The correct extension of coefficients in this case is to the field of Laurent series in $1/\hbar$, i.e. $\mathbb{C}[[1/\hbar]][\hbar]$, but this puts additional restrictions on the C_i in order for the star multiplication to be meaningful. It is sufficient that the star product (1) be *locally finite*, i.e., that for any $a, b \in \mathcal{A}$ only a finite number of the $C_i(a, b)$ be non-zero. (This is likewise frequently unmentioned but it is generally automatically satisfied when the C_i are bidifferential operators). The use of Laurent series in $1/\hbar$ rather than power series in \hbar has, as we will see, a profound effect on the structure of the resulting algebra.

If we set $C_0(a, b) = ab$, the original associative multiplication, then associativity of the star multiplication is equivalent to the condition that

$$\sum_{i+j=n} [C_i(C_j(a, b), c) - C_i(a, C_j(b, c))] = 0, \quad \text{all } n \geq 1; i, j \geq 0$$

for all a, b, c in the algebra \mathcal{A} . Transposing to the right side all terms with i or j equal to 0, this becomes

$$\begin{aligned} \sum_{i+j=n; i, j > 0} [C_i(C_j(a, b), c) - C_i(a, C_j(b, c))] = \\ aC_n(b, c) - C_n(ab, c) + C_n(a, bc) - C_n(a, b)c, \quad \text{all } n \geq 1. \end{aligned} \quad (2)$$

These are generally difficult conditions to meet. In the Hochschild cohomology theory, each C_i is a 2-cochain of \mathcal{A} with coefficients in itself, and the right side in (2) is the Hochschild coboundary of C_n . For $n = 1$ the left side is zero, so the coboundary of C_1 is zero, that is, C_1 is a 2-cocycle. This (or more properly, its cohomology class) is often called the *infinitesimal* of the deformation. A basic problem, given an infinitesimal deformation, is to construct a deformation which has it for infinitesimal. For $n = 2$ the left side of (2) is something constructed from C_1 which in fact will always be a 3-cocycle in the Hochschild theory, and the first requirement is that it be a coboundary, namely the coboundary of C_2 . Having C_1 and C_2 , the left side of (2) with $n = 3$ will again be a cocycle which is required to be a coboundary, and so forth for all n . Unless we have some control of the Hochschild cohomology of \mathcal{A} it is clear that the construction of deformations in such a step-by-step manner will not be easy.

Fortunately, there is one case in which all the conditions for associativity are automatically satisfied. A *derivation* D of \mathcal{A} is a linear mapping of \mathcal{A} into itself such that $D(ab) = (Da)b + a(Db)$. We have been careful with the order of the variables a and b here because the multiplication in the algebra \mathcal{A} need not have been commutative, although that is the case for any usual algebra of functions. Ordinary differentiation in the algebra of infinitely differentiable functions on \mathbb{R} is a derivation. Suppose that D' and D'' are commuting derivations of \mathcal{A} . Then the star multiplication defined by

$$a * b = ab + \hbar D' a D'' b + \frac{\hbar^2}{2!} D'^2 a D''^2 b + \frac{\hbar^3}{3!} D'^3 a D''^3 b + \dots$$

will be associative, cf. [3], something easily verified by direct computation. This (despite the consternation of mathematicians) is frequently written as

$$a * b = a e^{\hbar \overleftarrow{D'} \overrightarrow{D''}} b. \quad (3)$$

In the star product of (1) the C_n are then given by $C_n(a, b) = (1/n!) D'^n a D''^n b$. More generally, if $D'_1, \dots, D'_r, D''_1, \dots, D''_r$ are all mutually commuting derivations then

$$a * b = a e^{\hbar \sum_{i=1}^r \overleftarrow{D'_i} \overrightarrow{D''_i}} b$$

is again an associative multiplication.

A basic example illustrating (3) is that where $\mathcal{A} = \mathbb{C}[q, p]$, $D' = \partial_q$, $D'' = i\partial_p$. Then $q*p = qp + i\hbar$, while $p*q = pq$, so $[q, p]_* = q*p - p*q = i\hbar$. *The last equation determines the structure of the deformed algebra up to isomorphism but not the deformation* (which contains more information), as different deformations can give isomorphic algebras. In fact, referring to the basic equation (1), suppose that $T : \mathcal{A} \rightarrow \mathcal{A}$ is a linear map of the underlying vector space onto itself of the form $Ta = a + \hbar\tau_1 a + \hbar^2\tau_2 a + \dots$. Defining $a *' b = T^{-1}(Ta * Tb)$ and denoting by $\mathcal{A}_*, \mathcal{A}_{*}'$ the algebras with these two multiplications, the map T is an isomorphism $\mathcal{A}_{*}' \rightarrow \mathcal{A}_*$, so the new multiplication is also associative. We say that the deformations given by $*$ and $*'$ are *cohomologically equivalent* (c-equivalent), the adjective emphasizing that despite the isomorphism there may be some physical differences between the results. In particular, consider (3) and take $T = T_\lambda = e^{\lambda \hbar D' D''}$ where $D' D''$ is just the composite of the two derivations and λ is an arbitrary constant. Then it is easy to check that the resulting deformation is given by

$$a *_\lambda b = a e^{\hbar \overleftarrow{D'} \overrightarrow{D''} - \lambda \hbar (\overleftarrow{D'} \overrightarrow{D''} - \overleftarrow{D''} \overrightarrow{D'})} b \quad (4)$$

In particular, for $\lambda = 1/2$ we have

$$a *_{1/2} b = a e^{\frac{\hbar}{2} (\overleftarrow{D'} \overrightarrow{D''} - \overleftarrow{D''} \overrightarrow{D'})} b. \quad (5)$$

In the context of quantum theory, the deformation given by the commuting derivations D', D'' in (3) is generally called the ‘normal’ form, that obtained by interchanging D' and D'' or by setting $\lambda = 1$ in (4) is the ‘anti-normal’ form, and the skew symmetric form of (5) is the ‘Groenewold-Moyal’ form (GM)¹ [4, 7]. Historically, the fact that cohomologically equivalent deformations may not be physically equivalent immediately raised the problem of selecting from a family of c-equivalent deformations those which are physically meaningful. This was already addressed in [1] where one important reason cited for preferring the GM form is its greater symmetries. Another is homological: Every 2-cocycle of $\mathbb{C}[q, p]$ with coefficients in itself can be written uniquely as a sum of a symmetric part and a skew part. Both parts are again cocycles, but the symmetric part

¹While often attributed solely to Moyal, the basic idea is present earlier in the work of Groenewold, and anticipated even earlier in works of Wigner and Weyl.

is always a coboundary; there is, up to constant multiples, a unique skew 2-cocycle, and that cocycle is a biderivation, i.e., a derivation as a function of each argument. As mentioned, in the case of the simple harmonic oscillator our selection principle allows only the GM form, but like the foregoing principles (symmetry, cohomological uniqueness) our selection principle should apply to many other cases. (The normal and anti-normal forms are excluded in the case of a single oscillator but may be essential when one has infinitely many, as when quantizing a field, and one must normalize the lowest energy level of each to zero to avoid having that of the whole be infinite.)

Consider now the choice of coefficients of a deformed algebra. If we do not have some specific information about the 2-cochains C_i in (1) other than that they give a deformation (or about the derivations D' and D'' in (3) other than that they commute), then for coefficients one must take the power series ring $\mathbb{C}[[\hbar]]$, else the formulas will not be meaningful. In this classic approach some basic algebraic properties of \mathcal{A} are preserved. In particular, if a non-zero element a of \mathcal{A} is not a zero divisor in the original multiplication (i.e., if there is no $b \neq 0$ such that either $ab = 0$ or $ba = 0$) then a will not be a zero divisor in the deformed algebra. Similarly, if a was invertible then it will continue to be so. It follows that a deformation of an integral domain will continue to be an integral domain, and a deformation of a division ring (= skew field) will again be a division ring. A deformation of a unital algebra remains unital and the deformation will be, in fact, c -equivalent to one in which the original unit remains the unit. However, a deformation of a commutative algebra like $\mathbb{C}[q, p]$ need not remain commutative; this is the basis of quantization.

As mentioned, in a classical algebraic deformation we generally hope that the power series which are encountered actually converge for sufficiently small values of the deformation parameter \hbar , but for purely algebraic purposes this may not be necessary. Suppose now, however, that the deformation has the local finiteness property that for every a and b in the original (undeformed) algebra there is an N such that $C_i(a, b) = 0$ for all $i > N$. The deformed algebra will then already be defined over the polynomial ring $\mathbb{C}[\hbar]$, and we can extend coefficients, if we wish, to the field of Laurent series in $1/\hbar$. This is the case, for example, with $\mathcal{A} = \mathbb{C}[q, p]$ and $D' = \partial_q = \partial/\partial q, D'' = i\partial_p$ in (3). We must now also be careful in the definition of cohomological equivalence to require that T also be locally finite, i.e., that for all a there is an N such that $\tau_i(a) = 0$ for $i > N$. That is certainly the case for the T which gives the equivalence between the normal and Groenewold–Moyal deformations of $\mathbb{C}[q, p]$ (with $D' = \partial_q, D'' = \partial_p$).

When, in the locally finite case, we extend coefficients to Laurent series in $1/\hbar$ the structure of the deformed algebra may be very different from that obtained with power series as coefficients. What was before deformation an integral domain may acquire infinitely many orthogonal idempotents; as a result there may be no natural way to apply a contraction in the sense of İnönü and Wigner [6] to recover the original algebra. While this is inherent in deformation quantization, it raises difficult purely algebraic questions about the structure of the deformed algebra. The same is true, of course, of all algebras obtained by

c-equivalent deformations since they are all algebraically isomorphic.

2 Deformation quantization of the simple harmonic oscillator

The foundational paper [1] showed, in particular, that quantization of the simple harmonic oscillator could be viewed as an exercise in the deformation of the polynomial ring $\mathbb{C}[q, p]$, where now q and p are viewed as the position and momentum coordinates on the phase space \mathbb{R}^2 . The Hamiltonian function for the simple harmonic oscillator is

$$H(q, p) = \frac{p^2}{2m} + \frac{m\omega^2}{2}q^2. \quad (6)$$

In the classic approach to quantization one substitutes for q and p operators Q and P which satisfy the fundamental commutation relation $[Q, P] = i\hbar$. Generally this involves some ambiguity, for the Hamiltonian may contain monomials of positive degree simultaneously in p and q , but that is not a problem here. We can take, e.g., Q =multiplication by q , $P = -i\hbar\partial_q$ and with this seek solutions to the Schrödinger equation

$$i\hbar\dot{\psi} = H\psi.$$

This in effect chooses a specific *representation* of the Weyl algebra $\mathbb{C}\{q, p\}/(qp - pq - i\hbar)$ and with this choice ψ is viewed as a function of q and t . (The present H is time independent.) Mathematically this does not yet introduce any quantization; the latter is forced by the physical requirement that ψ be square integrable with absolute value tend to zero at $\pm\infty$. By contrast, *the deformation approach chooses a deformation which gives rise to the Weyl algebra*, e.g. that in (3) (i.e., such that the commutator of q and p is essentially their Poisson bracket) and rewrites the Schrödinger equation in the form

$$i\hbar\dot{\psi} = H * \psi. \quad (7)$$

This will be called the “deformation-Schrödinger” or d-Schrödinger equation.

Were H a matrix operating on a vector ψ , the solution would be $e^{-iHt/\hbar}\psi(0)$. Here, bearing in mind that H is now an element of a non-commutative algebra with multiplication $*$ one must still compute the exponential $\exp_*(-iHt/\hbar)$ where \exp_* indicates that the exponential must be computed using the deformed multiplication. The problem is to express the result, which is an element of the underlying vector space of the original (undeformed) algebra of functions on phase space, without reference to the deformed multiplication. There are now different possible choices for the deformed multiplication $*$ but $\exp_*(-iHt/\hbar)\psi(0)$ will always be a solution to the d-Schrödinger equation.

In deformation quantization generally, one knows from [1] that

$$\exp_*(-itH/\hbar) = \sum_E \pi_E e^{-itE/\hbar} \quad (8)$$

where the sum in the Fourier–Dirichlet series on the right is over the allowable energy levels E and the π_E are functions on the phase space which are orthogonal idempotents in the $*$ multiplication whose sum is 1. One has $H * \pi_E = E \pi_E$. (Note that we have tacitly extended coefficients to Laurent series in $1/\hbar$ and this has introduced zero-divisors into the new algebra.) Further, these idempotent functions when integrated over all of phase space will yield a common constant which, in the case of simple harmonic motion whose phase space is the q, p plane, is $2\pi\hbar$. We should like to interpret the π_E , which are functions on phase space, as giving a probability distribution there but in general they may take on negative values (depending on the deformation chosen). Although negative probabilities may not be directly observable, we shall see that at least in the case of simple harmonic motion a reasonable interpretation as probabilities may still be possible.

Following an idea often credited to Dirac, it is convenient to transform the Hamiltonian (6) into “holomorphic coordinates” by setting

$$a = \sqrt{\frac{m\omega}{2}}(q + i\frac{p}{m\omega}), \quad \bar{a} = \sqrt{\frac{m\omega}{2}}(q - i\frac{p}{m\omega}).$$

With this one has

$$H = \omega a \bar{a}.$$

The simplest deformation of $\mathbb{C}[a, \bar{a}]$ one can now choose is the normal form defined by setting

$$f *_N g = f e^{\hbar \overrightarrow{\partial_a \partial_{\bar{a}}}} g.$$

One then has $[a, \bar{a}]_{*_N} = \hbar$, which is equivalent to $[q, p]_{*_N} = i\hbar$. With this quantization we must compute $\exp_{*_N}(-iHt/\hbar) = \exp_{*_N}(-i\omega t a \bar{a}/\hbar)$. The d-Schrödinger equation (7) actually is a simple first order partial differential equation which shows, in particular, that the solution is a function of $a\bar{a}$ only. Writing $a\bar{a} = s$ and denoting the solution by $F(s, t)$, the d-Schrödinger equation becomes

$$i\hbar \partial_t F(s, t) = \omega s F(s, t) + \omega \hbar \partial_s F(s, t).$$

The required solution, which must have the value 1 at $t = 0$, is $F(s, t) = e^{-s/\hbar} \exp(e^{-i\omega t} s/\hbar)$, so we have

$$\exp_{*_N}(-i\omega t a \bar{a}/\hbar) = e^{-a\bar{a}/\hbar} \exp(e^{-i\omega t} a \bar{a}/\hbar),$$

where on the right one has the *ordinary* exponential. Expanding the expression on the right and writing $a\bar{a}/\hbar = H/\hbar\omega = \mu$, the coefficient of $e^{-in\omega t}$ becomes $e^{-\mu} \mu^n / n!$. Comparing with (8) we see that the allowable values for the energy are $E_n = n\hbar\omega$ and the corresponding $\pi_n^{(N)} = e^{-\mu} \mu^n / n!$ (where N indicates that the normal form is used). We will write the $\pi_n^{(N)}$ (and generally those which arise with any quantization) as functions of H with the latter viewed as the energy function on phase space. For any value of H the $\pi_n^{(N)}$ are just the terms in the classical Poisson distribution with mean $\mu = H/\hbar\omega$. This probability

distribution is sometimes called the ‘law of rare events’² : if μ is the mean number of events seen in unit time (or space) then the probability that in a given unit of time (or space) one will see exactly n events is $\pi_n^{(N)} = e^{-\mu} \mu^n / n!$. For example, if misprints are rare and the average number on a page is μ then the probability that a page will contain exactly n misprints is $e^{-\mu} \mu^n / n!$ (but μ may vary with the author). Unlike a Gaussian distribution, which depends on two parameters, its mean and standard deviation (‘uncertainty’ in physical terms, square root of its variance), the Poisson has but one, its mean. The variance is identical with its mean and the standard deviation is the square root of its mean. For large values of the mean, the distribution resembles a Gaussian with mean μ and standard deviation $\sqrt{\mu}$.

The question is how to interpret the appearance of the Poisson distribution here, bearing in mind that we have somehow the ‘wrong’ quantization (or at least not that in textbooks, since the lowest allowable energy is precisely zero, not $\hbar\omega/2$). We will see that this quantization essentially presumes that we know the mean energy of the oscillator precisely, something which is not physically possible. In that impossible case it seems to say that if the mean energy is μ then the probability that the oscillator will be observed in a state with the quantum number n is $\pi_n^{(N)} = e^{-\mu} \mu^n / n!$. But note that even though we have the ‘wrong’ minimal energy, the spectrum here is simply shifted by $\hbar\omega/2$ from the textbook case, so the differences between allowable energy levels, which determine the spectrum, coincide with the usual. Nevertheless, the normal form of quantization is excluded by our selection principle. For with it all true probability distributions of energy are observable including a delta function, which has zero uncertainty, while the quantum uncertainty is always positive. (In fact, we will see that when the normal form is viewed as a limit the initial energy distribution is a delta function.)

It is easy to verify that the $\pi_n^{(N)}$ are orthogonal idempotents in the $*_N$ multiplication, summing to 1 and having a fixed common integral over phase space: Direct computation shows that the integral of each is $2\pi\hbar$ independent of n . That $\sum_{n=0}^{\infty} \pi_n^{(N)} = 1$ follows simply from setting $t = 0$. Finally, one way to see that the $\pi_n^{(N)}$ are orthogonal idempotents is to observe that although $*_N$ is a non-commutative multiplication, the $\pi_n^{(N)}$ and $\exp_{*_N}(-i\omega t a \bar{a} / \hbar)$ are all functions only of the single element $a \bar{a}$ and hence all commute. Comparing the expansions of the two sides of the equation $\exp_{*_N}(-i\omega t a \bar{a} / \hbar) *_N \exp_{*_N}(-i\omega t a \bar{a} / \hbar) = \exp_{*_N}(-2i\omega t a \bar{a} / \hbar)$ will show that $\pi_0^{(N)}$ is idempotent. Denoting it for the moment by e , we clearly have for any idempotent e that $e(1 - e) = 0$, and that $1 - e$ is again idempotent. Proceeding by induction will show that the $\pi_n^{(N)}$ are all mutually orthogonal idempotents.

While the normal form of deformation has been excluded by our selection principle, it already raises an interesting algebraic question equally meaningful

²Curiously, it arose neither from gambling nor physics but from Siméon-Denis Poisson’s study of the French judicial process in his “Recherches sur la probabilité des jugements en matière criminelle et matière civile”, 1837

for all c-equivalent deformations. For the moment, let \mathcal{A} denote the polynomial ring $\mathbb{C}[q, p]$ and let \mathcal{A}_\hbar denote the algebra to which we have deformed it. Note that as long as coefficients are restricted to polynomials in \hbar it is meaningful to let $\hbar \rightarrow 0$ in order to recover the original algebra; this gives the (only) correct statement of the correspondence principle. The resulting algebra is essentially the first Weyl algebra, a simple algebra (i.e., one without proper two-sided ideals) whose cohomology with coefficients in itself vanishes in all positive dimensions, in particular in dimension 2, and which is therefore rigid. With coefficients extended to $\mathbb{C}[[1/\hbar]][\hbar]$ recovery of the original algebra by letting $\hbar \rightarrow 0$ is no longer possible. We have an algebra in which the identity has decomposed into a direct sum of infinitely many orthogonal idempotents e_1, e_2, \dots and whose precise structure we no longer know. The theorem that there is no degeneracy in one dimension suggests that each $e_i \mathcal{A}_\hbar e_i$ has dimension 1 and that the same is probably true for all $e_i \mathcal{A}_\hbar e_j$. The simplest conjecture concerning structure would be that in each $e_i \mathcal{A}_\hbar e_j$ we can choose an element e_{ij} with $e_{ii} = e_i$ and $e_{ij} e_{jk} = e_{ik}$, and that the algebra consists of linear combinations of these (but what beside the finite ones may be allowed is not clear). Again, the same question arises for all c-equivalent deformations of $\mathbb{C}[q, p]$.

3 Quantizations with $\lambda \neq 0$

Following the prescription in § 1, we now set $T_\lambda = e^{\lambda \hbar D' D''}$ and define

$$f *_\lambda g = T_\lambda^{-1} (T_\lambda f *_{\mathcal{N}} T_\lambda g) = f e^{\hbar((1-\lambda)\vec{\partial}_a \vec{\partial}_{\bar{a}} - \lambda \vec{\partial}_{\bar{a}} \vec{\partial}_a)} g.$$

There are now several approaches to computing $\exp_{*_\lambda}(-iHt/\hbar)$. One can use the first equality above to get expressions for the quantities which we will now denote by $\pi_n^{(\lambda)}$, where $\pi_n^{(0)} = \pi_n^{(N)}$; this will give them all in the form of power series. The second approach, which we adopt, is to use only the value obtained for $\pi_0^{(\lambda)}$ from the first method and then to adapt the procedure in [5, Appendix] to compute $\exp_{*_\lambda}(-iHt/\hbar)$. The third approach is to note, as in the preceding section, that $\exp_{*_\lambda}(-iHt/\hbar)$ will be a function only of $a\bar{a}$; denoting this again by s and the result by $F(s, t)$ one can solve the partial differential equation (now of second order in s) which F satisfies. However, we will see that one can also effectively solve the differential equation in closed form once closed expressions for the $\pi_n^{(\lambda)}$ have been obtained from the second method by using the generating function for the Laguerre polynomials. Since $T_\lambda a\bar{a} = a\bar{a} + \hbar\lambda$, with the first approach we have

$$\begin{aligned} \exp_{*_\lambda}(-iHt/\hbar) &= T_\lambda^{-1} \exp_{*_{\mathcal{N}}}(-i\omega t T_\lambda(a\bar{a}/\hbar)) \\ &= e^{-\lambda \hbar \partial_a \partial_{\bar{a}}} \exp_{*_{\mathcal{N}}}(-i\omega t(a\bar{a}/\hbar + \lambda)) \\ &= e^{-\lambda i\omega t/\hbar} e^{-\lambda \partial_a \partial_{\bar{a}}} e^{-a\bar{a}/\hbar} \exp(e^{-i\omega t} a\bar{a}/\hbar) \\ &= e^{-\lambda i\omega t/\hbar} e^{-\lambda \partial_a \partial_{\bar{a}}} \exp((e^{-i\omega t} - 1)a\bar{a}/\hbar). \end{aligned}$$

A simple computation using the definition of the Laguerre polynomials then shows that

$$\exp_{*\lambda}(-iHt/\hbar) = e^{-\lambda i\omega t} \sum_{k=0}^{\infty} (-\lambda)^k (e^{-i\omega t} - 1)^k L_k(a\bar{a}/\lambda\hbar)$$

where L_k is the k th Laguerre polynomial. We may now replace $a\bar{a}/\hbar$ on the right with $H/\hbar\omega$ since the computations on the right now all take place in the undeformed algebra. Expanding the right side then gives

$$\exp_{*\lambda}(-iHt/\hbar) = \sum_{n=0}^{\infty} (-1)^n \sum_{k=0}^{\infty} \lambda^k \binom{k}{n} L_k(H/\lambda\hbar\omega) e^{-i(n+\lambda)\omega t}.$$

The spectrum has thus been shifted, the allowable values of the energy are now $E = (n + \lambda)\hbar\omega$, and we have

$$\pi_n^{(\lambda)} = (-1)^n \sum_{k=0}^{\infty} \lambda^{n+k} \binom{n+k}{k} L_{n+k}(H/\lambda\hbar\omega),$$

which can be negative for some H . Using the generating function for the Laguerre polynomials,

$$\frac{1}{1+x} \exp\left(\frac{zx}{1+x}\right) = \sum_{k=0}^{\infty} x^k (-1)^k L_k(z),$$

the special case $n = 0$ gives

$$\pi_0^{(\lambda)} = \sum_{k=0}^{\infty} \lambda^k L_k\left(\frac{H}{\lambda\hbar\omega}\right) = \frac{1}{1-\lambda} \exp\left(-\frac{H}{(1-\lambda)\hbar\omega}\right).$$

We can now adapt the procedure in [5, Appendix] to get from this the closed form for all the $\pi_n^{(\lambda)}$, namely

$$\pi_n^{(\lambda)} = \frac{1}{1-\lambda} \left(\frac{-\lambda}{1-\lambda}\right)^n L_n\left(\frac{H}{\lambda(1-\lambda)\hbar\omega}\right) \exp\left(-\frac{H}{(1-\lambda)\hbar\omega}\right).$$

Letting $\lambda \rightarrow 0$ recovers original Poisson distribution. Comparing the two expressions for $\pi_n^{(\lambda)}$ gives the following identity involving Laguerre polynomials:

$$\begin{aligned} (-1)^n \sum_{k=0}^{\infty} \lambda^{n+k} \binom{n+k}{k} L_{n+k}\left(\frac{z}{\lambda}\right) \\ = \frac{1}{1-\lambda} \left(\frac{-\lambda}{1-\lambda}\right)^n L_n\left(\frac{z}{\lambda(1-\lambda)}\right) \exp\left(-\frac{z}{(1-\lambda)}\right). \end{aligned} \tag{9}$$

(Setting $\lambda = 1/2$ and $z = 0$ this asserts, for example, that $\sum_k (1/2)^{n+k} \binom{n+k}{k} = 2$ independent of n , something easily verified directly.) Multiplying the left side

by $e^{-z/\lambda}L_m(z/\lambda) = e^{-z/\lambda}L_m((1-\lambda)z/\lambda(1-\lambda))$ and integrating, the orthogonality relations of the Laguerre polynomials together with an obvious change of variables gives

$$\int_0^\infty L_m((1-\lambda)z)L_n(z)e^{-z}dz = \begin{cases} \binom{m}{n}\lambda^m\left(\frac{1-\lambda}{\lambda}\right)^n & \text{if } m \geq n \\ 0 & \text{otherwise} \end{cases}.$$

Replacing λ by $1-\lambda$ and comparing the coefficients of the powers of λ on the two sides gives the coefficients in the Fourier-Laguerre expansion of z^k :

$$\int_0^\infty z^k L_n(z)e^{-z}dz = \begin{cases} (-1)^n \binom{k}{n} k! & \text{if } k \geq n \\ 0 & \text{if } k < n \end{cases}. \quad (10)$$

This fundamental result, which will show the existence of enough observable distributions, can also be derived in an elementary way, since it is just the formula for the change of basis from the Laguerre polynomials to the powers of x in the vector space of polynomials in x : Let A be the infinite lower triangular matrix with rows and columns indexed by $0, 1, 2, \dots$ and (i, j) entry equal to $(-1)^j \binom{i}{j}$, and D be the infinite diagonal matrix with diagonal entries $1/n!$, $n = 0, 1, 2, \dots$. Letting X be the infinite column vector $(1, x, x^2, x^3, \dots)^t$, the n th entry in the vector $L = ADX$ is just the Laguerre polynomial $L_n(x)$. To write X in terms of L it is sufficient therefore to invert AD , the only problem being the inversion of A . However, A is equal to its own inverse, for writing $x^r = (1 - (1-x))^r = \sum_i (-1)^i \binom{r}{i} (1-x)^i$ gives

$$\sum_i (-1)^i \binom{r}{i} (-1)^j \binom{i}{j} = \begin{cases} 1 & \text{if } j = r \\ 0 & \text{otherwise} \end{cases}.$$

Therefore $X = D^{-1}AL$, which is precisely what (10) asserts.

While k is an integer in (10), one can deduce more generally that

$$\int_0^\infty z^p L_n(z)e^{-z}dz = (-1)^n \frac{\Gamma(p+1)^2}{n! \Gamma(p-n+1)}.$$

With (9), the generating function for the Laguerre polynomials gives the following closed form for the $*_\lambda$ exponential of $-iHt/\hbar$,

$$\exp_{*\lambda}(-iHt/\hbar) = \frac{e^{-i\lambda\omega t}}{1-\lambda+\lambda e^{-i\omega t}} \exp\left(\frac{2H}{\hbar\omega} \cdot \frac{e^{-i\omega t}-1}{1-\lambda+\lambda e^{-i\omega t}}\right);$$

at $\lambda = 1/2$ one recovers the known formula for the Groenewold-Moyal case,

$$\exp_{*1/2}(-iHt/\hbar) = \frac{1}{\cos(\omega t/2)} \exp\left(\frac{2H}{-i\hbar\omega} \tan(\omega t/2)\right).$$

The only values of λ that need to be considered are $0 \leq \lambda \leq 1/2$. Setting $t = 0$ shows that $\sum \pi_n^{(\lambda)} = 1$ for any value of λ ; that the $\pi_n^{(\lambda)}$ are mutually orthogonal idempotents follows exactly as in the case $\lambda = 0$. We could, of course also deduce

this from the fact that the $\pi_n^{(\lambda)}$ are the transforms of the π_n^N by T_λ , but writing, as before, $\mu = H/\hbar\omega$ we also have the duality relation

$$\int_0^\infty \pi_n^{(\lambda)}(\mu) \pi_m^{(1-\lambda)}(\mu) d\mu = \delta_{n,m}.$$

The Groenewold-Moyal case ($\lambda = 1/2$) is self-dual.

4 Negative probabilities and basic observable distributions

Returning to the question of negative probabilities, unlike the $\pi_n^{(N)}$, we can not view the $\pi_n^{(\lambda)}$ as giving an ordinary probability distribution over the energy values H since for all $n > 0$ and any positive λ , $\pi_n^{(\lambda)}$ will be negative for some positive value of H . (Moreover, we conjecture that for any fixed $\lambda \neq 0, 1$ and arbitrary $H > 0$ there must be an $n > 0$ such that $\pi_n^{(\lambda)} < 0$; this is easily seen to be true for sufficiently small H since $\pi_0^{(\lambda)}(0) = 1/(1-\lambda) > 0$ and $\sum_{n=0}^\infty \pi_n^{(\lambda)} = 1$ for all H . In fact, while the foregoing sum is absolutely convergent for $\lambda < 1/2$ it is only conditionally convergent at the Groenewold-Moyal limit $\lambda = 1/2$, and the convergence there is very slow.)

Negative probabilities can not be dismissed as fiction. In the present case, accepting them at face value gives the correct expected value for the energy: differentiating the basic equation (8) with respect to time and setting $t = 0$ gives

$$H = \sum \pi_E E,$$

independent of the form of deformation. (Differentiating twice will give the quantum second moment rather than that of the original distribution, since the left side at $t = 0$ will be $H * H$.) In what remains we again write μ for the dimensionless quantity $H/\hbar\omega$ when it is viewed as an ordinary scalar.

As remarked at the beginning, one view of negative probabilities is that while they can not be observed directly we can observe positive distributions derived from them and thereby indirectly conclude their existence. Suppose that in our observation of the harmonic oscillator we have a true probability distribution $p(\mu)$ for the energy, that is, one which is non-negative, defined for $\mu \geq 0$, and has $\int_0^\infty p(\mu) d\mu = 1$. With this, the probability of the oscillator being observed at the n th energy level becomes $\pi_n^{(\lambda)}(\mu, p) = \int_0^\infty \pi_n^{(\lambda)}(\mu) p(\mu) d\mu$. For some probability distributions p these will all be non-negative; such p have been called observable distributions. The existence of sufficiently many is given immediately by (10), for writing

$$p_k^{(\lambda)}(\mu) = \frac{1}{\lambda k!} \left(\frac{\mu}{\lambda}\right)^k e^{-\frac{\mu}{\lambda}}$$

one has from (10) that

$$\int_0^\infty \pi_n^{(\lambda)}(\mu) p_k^{(\lambda)}(\mu) d\mu = \begin{cases} \binom{k}{n} \lambda^n (1-\lambda)^{k-n} & \text{if } k \geq n \\ 0 & \text{if } k < n \end{cases}.$$

The $p_k^{(\lambda)}$ are thus observable distributions. The coefficients on the right are the Fourier-Laguerre coefficients of the distribution (relative to the deformation with parameter λ). We will call the $p_k^{(\lambda)}$ *basic* observable distributions since suitable (in fact unique) linear combinations of them (necessarily involving negative coefficients) give all distributions with but a single non-zero Fourier-Laguerre coefficient (i.e., we can recover those given by the individual $\pi_n^{(\lambda)}$). The basic observable distributions are the extreme elements of the convex cone of observable distributions and they span that cone. Note that the basic distributions have only a finite number of non-zero Fourier-Laguerre coefficients.

5 The uncertainty inequality

It is a classic computation that with the distribution $p_k^{(\lambda)}$ the mean or expected value of μ , namely $\int \mu p_k^{(\lambda)}(\mu) d\mu$, is just $\lambda(k+1)$. This is the mean value of the energy with the basic observable distribution $p_k^{(\lambda)}$. (Note that its minimum at $k=0$ is, as expected, just λ .) The second moment of the distribution is

$$\int \mu^2 p_k^{(\lambda)}(\mu) d\mu = \lambda^2(k+1)(k+2).$$

It follows that the variance is $\lambda^2(k+1)$, the square root of which is the standard deviation or ‘uncertainty’. The other evaluation of the expected energy in $p_k^{(\lambda)}$ necessarily gives the same result, for as observed earlier the energy calculation is independent of the quantization (and uses the negative probabilities). In fact, we have

$$\sum_{n=0}^{\infty} \int_0^{\infty} (n+\lambda) \pi_n^{(\lambda)}(\mu) p_k^{(\lambda)}(\mu) d\mu = \sum_{n=0}^k (n+\lambda) \binom{k}{n} \lambda^n (1-\lambda)^{k-n} = (k+1)\lambda.$$

Note that if we try to keep the mean of the distribution constant while letting λ tend to zero, then the deformation becomes the normal one and the distribution becomes a Dirac delta supported at the mean energy. This is what was meant earlier by saying that the normal form of quantization assumes that the energy is precisely known.

We can now apply our selection principle. With the basic observable distribution $p_k^{(\lambda)}$ one has

$$\begin{aligned} \sum_{n=0}^{\infty} \int_0^{\infty} (n+\lambda)^2 \pi_n^{(\lambda)}(\mu) p_k^{(\lambda)}(\mu) d\mu &= \sum_{n=0}^k (n+\lambda)^2 \binom{k}{n} \lambda^n (1-\lambda)^{k-n} \\ &= (k^2 + k + 1)\lambda^2 + k\lambda. \end{aligned}$$

The variance now is $k\lambda(1-\lambda)$. By our selection principle, which asserts, in particular, that quantization should not increase uncertainty, this quantum variance

must be smaller than the previous distribution variance. One therefore has the inequality

$$k\lambda(1-\lambda) < (k+1)\lambda^2.$$

We may not only assume that λ is strictly positive, but as observed earlier, that $0 < \lambda \leq 1/2$, so this implies that

$$\lambda > \frac{k}{2k+1}.$$

This being true for all non-negative k it follows that we must have $\lambda = 1/2$, leaving the Groenewold-Moyal form as the only one consistent with the selection principle. Similar arguments may apply more generally to select one quantization from a family of cohomologically equivalent ones.

Finally, fixing λ at $1/2$, note that the variance of the distribution $p_k^{(1/2)}$ is $(k+1)/4$ while its quantum variance is $k/4$, so the difference in variances is always just $1/4$. The difference in uncertainties, however, is $(\sqrt{k+1} - \sqrt{k})/2$ which tends to 0 as the mean energy increases. This does not hold for any λ strictly between 0 and $1/2$, so for the simple harmonic oscillator it would be sufficient to require of a quantization procedure that as energy tends to infinitely (and quantization becomes unnoticeable) the difference in uncertainties tends to zero, but this might not be a sufficiently strong selection principle in general.

References

- [1] F. Bayen, M. Flato, C. Frönsdal, A. Lichnerowicz, and D. Sternheimer. Deformation theory and quantization I,II. *Ann. Phys. (NY)*, 111:61–110,111–151, 1978.
- [2] P. Bonneau, M. Gerstenhaber, A. Giaquinto, and D. Sternheimer. Quantum groups and deformation quantization: Explicit approaches and implicit aspects. *J. Math. Phys.*, 45:3703–3741, 2004.
- [3] M. Gerstenhaber. On the deformation of rings and algebras. *Ann. of Math.*, 79:59–103, 1964.
- [4] H. J. Groenewald. On the principles of elementary quantum mechanics. *Physica*, 12:405–460, 1946.
- [5] A. C. Hirshfeld and P. Henselder. Deformation quantization in the teaching of quantum mechanics. *Am. J. Physics*, 70:537–547, 2002. Also at [arXiv:quant-ph/0208163](https://arxiv.org/abs/quant-ph/0208163) v1.
- [6] E. İnönü and E. P. Wigner. On the contraction of groups and their representations. *Proc. Nat. Acad. Sci. USA*, 39:510–524, 1953.
- [7] J. E. Moyal. Quantum mechanics as a statistical theory. *Proc. Cambridge Philosophical Soc.*, 45:99–124, 1949.